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Algebraic structure of stochastic expansions and efficient simulation

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Abstract We investigate the algebraic structure underlying the stochastic Taylor solution expansion for stochastic differential systems. Our motivation is to construct *efficient* integrators. These are approximations that generate strong numerical integration schemes that are more accurate than the corresponding stochastic Taylor approximation, independent of the governing vector fields and to all orders. The sinhlog integrator introduced by Malham & Wiese (2009) is one example. Herein we: show that the natural context to study stochastic integrators and their properties is the convolution shuffle algebra of endomorphisms; establish a new whole class of efficient integrators; and then prove that, within this class, the sinhlog integrator generates the *optimal* efficient stochastic integrator at all orders.

Keywords stochastic simulation · convolution shuffle algebra · efficient integrators

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1 Introduction

We consider the simulation of stochastic differential systems of arbitrary order $N \in \mathbb{N}$. We assume for $y_t \in \mathbb{R}^N$ our system has the form

$$y_t = y_0 + \sum_{i=0}^d \int_0^t V_i(y_\tau) dW_\tau^i.$$

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This system is driven by a d -dimensional Wiener process (W^1, \dots, W^d) and governed by a drift vector field V_0 and diffusion vector fields V_1, \dots, V_d . We use the convention $W_t^0 \equiv t$ and interpret the stochastic integrals in the Stratonovich sense. Hereafter we will assume $t \in \mathbb{R}_+$ lies in the interval of existence of the solution. In general, we also suppose that the vector fields $V_i: \mathbb{R}^N \rightarrow \mathbb{R}^N$ for $i = 0, \dots, d$ are sufficiently smooth and non-commuting. We focus on solution series and their use in strong simulation schemes. The stochastic Taylor expansion for the flowmap $\varphi_t: y_0 \mapsto y_t$, taking the data y_0 at time $t = 0$ to the solution y_t at time t for the stochastic differential system above, is given by (see for example Baudoin 2004 or Lyons & Victoir 2004)

$$\varphi_t = \sum_w J_w(t) V_w.$$

Here $w = a_1 \dots a_n$ is a word with letters a_1, \dots, a_n chosen from the alphabet $\mathbb{A} := \{0, 1, \dots, d\}$. The sum is over all possible words w in \mathbb{A}^* , the free monoid on \mathbb{A} . All the stochastic information is encoded in the scalar random variables (Stratonovich integrals)

$$J_w(t) := \int_0^t \dots \int_0^{\tau_{n-1}} dW_{\tau_n}^{a_1} \dots dW_{\tau_1}^{a_n}.$$

The partial differential operators $V_w := V_{a_1} \circ \dots \circ V_{a_n}$, constructed by composing the vector fields, encode all the geometric information.

Strong numerical integration schemes for stochastic differential systems are based on truncating the stochastic Taylor expansion and applying the resulting approximate flowmap over successive small computation subintervals spanning the global time interval of interest. More generally, across a computation interval $[0, t]$, for any smooth map $f: \text{Diff}(\mathbb{R}^N) \rightarrow \text{Diff}(\mathbb{R}^N)$, we can:

1. Construct the series $\sigma_t = f(\varphi_t)$;
2. Truncate the series σ_t to $\hat{\sigma}_t$ according to a grading $g(w)$ on the words w ;
3. Compute $\hat{\varphi}_t = f^{-1}(\hat{\sigma}_t)$ and use this as the basis of a numerical scheme.

For example, suppose $f = \text{id}$, the identity map. Then σ_t is just the stochastic Taylor expansion φ_t , which we split according to the grading $g(w)$ as follows

$$\varphi_t = \sum_{g(w) \leq n} J_w V_w + \sum_{g(w) \geq n+1} J_w V_w,$$

for $n \in \mathbb{N}$. A stochastic Taylor numerical scheme of strong order $n/2$ would be the first term on the right shown; the remainder is the last term. The grading $g(w)$ here is determined by the variance of the stochastic integrals J_w ; zero letters in w contribute a count of one while non-zero letters contribute a count of one-half towards $g(w)$. An important technicality is to include in the integrator, the *expectation* of the terms in the remainder at leading order. This is because not including them would decrease the expected global order by one-half (an explanation can be found in Buckwar, Malham & Wiese 2012 or Malham & Wiese 2009). In other words, a stochastic Taylor integrator of strong order $n/2$ is

$$\hat{\varphi}_t = \sum_{g(w) \leq n} J_w V_w + \sum_{g(w) = n+1} \bar{E}(J_w) V_w,$$

where the expectations of the J_w , here denoted $\bar{E}(J_w)$, are known analytically. The *Euler–Maruyama* and *Milstein* numerical methods correspond to the cases $n = 1$ and $n = 2$, respectively, applied on successive computation subintervals with the vector fields evaluated on the initial data on each subinterval. Stochastic Runge–Kutta methods are constructed by replacing the partial differential operators V_w by finite differences.

Another example is $f = \log$ so that $\sigma_t = \log \varphi_t$. This is the exponential Lie series which is the basis of the Castell–Gaines method (see Castell & Gaines 1995, 1996; also see Azencott 1982, Ben Arous 1989 and Castell 1993). Truncating the exponential Lie series to $\hat{\sigma}_t$ generates a Lie polynomial in the Lie algebra of vector fields. We assume we can suitably approximately simulate the multiple integrals J_w retained in the truncation (more on this presently). Hence $\hat{\varphi}_t = \exp \hat{\sigma}_t$ and our approximation \hat{y}_t to the solution y_t across $[0, t]$ can be generated as follows. For a given realization of the J_w terms retained, we simply solve the ordinary differential system $u' = \hat{\sigma}_t \circ u$ for $u = u(\tau)$, for $\tau \in [0, 1]$ and $u(0) = y_0$. Though we might achieve this analytically, more often one has to use a suitably accurate ordinary differential integrator. In either case we have $u(1) \approx \hat{y}_t$.

We measure the accuracy of a strong order integrator by the root-mean-square of its local remainder

$$r_t := \varphi_t - \hat{\varphi}_t.$$

More precisely, we measure $\|r_t \circ y_0\|_{L^2}$ for each $y_0 \in \mathbb{R}^N$, i.e. the square-root of the expectation of the Euclidean norm of $r_t \circ y_0$. Let us now clarify an important issue. The order of a strong numerical method is determined by the set of multiple Wiener integrals simulated and included. Since the set of all multiple (Stratonovich) Wiener integrals is generated by those based on Lyndon words (see Reutener 1993, p. 111 and Gaines 1994), we need only simulate the multiple Wiener integrals indexed by Lyndon words. The other multiple Wiener integrals of that order can be computed by linear combinations of products of the appropriate Lyndon word multiple integrals of that order or less. However Lyndon word multiple integrals of the same order cannot be generated as such (or from each other). Hence more correctly, the order of a method is determined by the set of Lyndon word multiple Wiener integrals included. Consequently, in general with this multiple integral set, a more accurate method can only have a better error constant and an improvement in order scaling is not possible. Throughout this article we assume we can suitably approximate/simulate the Lyndon word multiple Wiener integrals up to the order required. The bulk of computational effort in higher order strong simulation methods is devoted to this task, though there has been some recent advances on this front; see Wiktorsson (2001), Lyons and Victoir (2004), Levin & Wildon (2008) and Malham & Wiese (2011).

Castell & Gaines (1995, 1996) proved that their simulation method of strong order one-half was *asymptotically efficient* in the sense of Newton (1991): it “minimizes the leading coefficient in the expansion of the mean-square errors as power series in the sample step-size”. This property extends to their strong order one method when the diffusion vector fields commute. However, Malham & Wiese (2009) demonstrated that when the stochastic differential system above is driven by a multi-dimensional driving Wiener process and the governing diffusion vector fields do not commute, then a strong numerical simulation based on the exponential Lie series is not asymptotically efficient (independent of the vector fields);

also see Lord, Malham & Wiese (2008). Malham & Wiese (2009) proved, in the absence of drift, that a strong simulation method generated by taking the sinhlog of the flowmap, truncating the resulting series and then taking the inverse sinhlog, is *efficient* to all orders. This means that the error of the sinhlog integrator is always smaller than the error of the corresponding stochastic Taylor integrator in the mean-square sense, independent of the vector fields. In this paper we:

1. Show that the natural context to study stochastic integrators and their properties is the convolution algebra of endomorphisms on the Hopf shuffle algebra of words;
2. Establish a new class of efficient stochastic integrators using this algebraic structure (we include drift and grade according to word length);
3. Prove that within this class, the sinhlog integrator generates the *optimal* efficient stochastic integrator to all orders. By this we mean that the error of the integrator realizes its smallest possible value compared to the error of the corresponding stochastic Taylor integrator, in the mean-square sense.

Our paper is structured as follows. In §2 we demonstrate the direct relation between stochastic expansions and the convolution shuffle algebra of endomorphisms on the Hopf shuffle algebra of words. We define an inner product structure on the convolution shuffle algebra of endomorphisms that is based on the correlation measure between multi-dimensional stochastic processes in §3. We also demonstrate some natural useful identities and orthogonality properties of endomorphisms therein. In §4 we prove results 2 and 3 stated above. Finally in §5 we discuss the implications of our results and provide some concluding remarks.

2 Stochastic expansions and the convolution shuffle algebra

We introduce the convolution shuffle algebra and show it is the natural context to study stochastic expansions. For the moment, we proceed formally as the basic material can be found in the monograph by Reutenauer (1993); also see Remark 1 below. Dropping J 's and V 's, we can represent the stochastic Taylor series for the flowmap by

$$\varphi = \sum_w w \otimes w,$$

which lies in the product algebra $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$ over the commutative ring $\mathbb{K} = \mathbb{R}$. We are interested in the following two Hopf algebra structures on $\mathbb{K}\langle\mathbb{A}\rangle$. One has shuffle \sqcup as product and deconcatenation Δ as coproduct ($\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ on the left). The other has concatenation as product and deshuffle as coproduct ($\mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$ on the right). The unit, counit and antipode are the same for both algebras $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ and $\mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$. We denote the empty word $\mathbf{1} \in \mathbb{K}\langle\mathbb{A}\rangle$. The product of two terms in $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$ is

$$(u \otimes x)(v \otimes y) = (u \sqcup v) \otimes (xy),$$

where we concatenate the words on the right representing the composition of vector fields. On the left, $u \sqcup v$ represents the sum of all possible shuffles of the words u and v , representing the product of two multiple integrals.

Remark 1 The homomorphism from $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$ to the free associative algebra of vector fields is established as follows (see Malham & Wiese 2009, Section 2(c)). Let \mathbb{J} denote the ring generated by multiple Stratonovich integrals and the constant random variable 1, with pointwise multiplication and addition. Also let \mathbb{V} denote the set of all vector fields on \mathbb{R}^N . The flow map φ defined in the introduction lies in $\mathbb{J}\langle\mathbb{V}\rangle \cong \bigoplus_{n \geq 0} \mathbb{J} \otimes \mathbb{V}_n$, where \mathbb{V}_n is the subset of vector fields V_w with w of length n . The linear *word-to-vector field map* $\kappa: \mathbb{R}\langle\mathbb{A}\rangle \rightarrow \mathbb{V}$ given by $\kappa: w \mapsto V_w$ is a concatenation homomorphism, i.e. $\kappa(uv) = \kappa(u)\kappa(v)$ for any $u, v \in \mathbb{A}^*$. And the linear *word-to-integral map* $\mu: \mathbb{R}\langle\mathbb{A}\rangle \rightarrow \mathbb{J}$ given by $\mu: w \mapsto J_w$ is a shuffle homomorphism, i.e. $\mu(u \sqcup v) = \mu(u)\mu(v)$ for any $u, v \in \mathbb{A}^*$ (see Lyons, et. al. 2007, p. 35 or Reutenauer 1993, p. 56; this also underlies our choice to use Stratonovich integrals rather than Itô integrals which satisfy a quasi-shuffle relation). Hence the map $\mu \otimes \kappa: \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}} \rightarrow \bigoplus_{n \geq 0} \mathbb{J} \otimes \mathbb{V}_n$ is a Hopf algebra homomorphism which naturally extends to the free associative algebra of vector fields.

Suppose we apply a polynomial or power series function to the flow-map φ , say $f = f(\varphi)$. For example suppose f has a simple power series expansion

$$f(\varphi) = \sum_{k=0}^{\infty} c_k \varphi^k$$

with coefficients $\{c_n \in \mathbb{K}: n \geq 0\}$. Then the product in $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$ implies that after rearrangement, we can always express the result in the form

$$f(\varphi) = \sum_{w \in \mathbb{A}^*} (F \circ w) \otimes w,$$

where $F \in \text{End}(\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}})$ is given by ($|w|$ denotes the length of the word)

$$F \circ w = \sum_{k=0}^{|w|} c_k \sum_{\substack{u_1, \dots, u_k \in \mathbb{A}^* \\ w=u_1 \dots u_k}} u_1 \sqcup \dots \sqcup u_k.$$

See Reutenauer (1993, p. 58) or Malham and Wiese (2009) for more details. This suggests we can encode the action of any such function f of the flowmap φ by an endomorphism $F \in \text{End}(\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}})$. Indeed the embedding $\text{End}(\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}) \rightarrow \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$ given by

$$X \mapsto \sum_w X(w) \otimes w,$$

is an algebra homomorphism for the non-commutative convolution product defined for all $X, Y \in \text{End}(\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}})$ by

$$X \star Y = \sqcup \circ (X \otimes Y) \circ \Delta.$$

Since the coproduct Δ here is deconcatenation, which takes a word w and produces a sum of all possible two-partitions $u \otimes v$ of w , we see that explicitly

$$(X \star Y)(w) = \sum_{\substack{u, v \in \mathbb{A}^* \\ w=uv}} X(u) \sqcup Y(v).$$

Thus, we can encode and study the structure and properties of functions of the flowmap through endomorphisms $F \in \text{End}(\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}})$, with convolution as product. For convenience, we henceforth denote

$$\mathbb{H} := \text{End}(\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}),$$

the convolution shuffle algebra of endomorphisms on $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$, which is a unital associative non-commutative \mathbb{K} -algebra. The unit ν in \mathbb{H} is the composition of the unit and counit. Indeed ν sends non-empty words to 0 and the empty word to itself. For any Hopf algebra, by definition the antipode S is the inverse of the identity endomorphism with respect to the convolution. Thus we have

$$S \star \text{id} = \text{id} \star S = \nu.$$

On $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ the antipode $S \in \mathbb{H}$ is given by $S(a_1 \dots a_n) := (-1)^n a_n \dots a_1$, i.e. it is the sign-reversing endomorphism.

Remark 2 There is a dual convolution concatenation algebra which we could alternatively utilize; see Reutenauer (2009; Section 1.5).

Remark 3 There is natural compatibility between convolution and composition in \mathbb{H} . For an algebra homomorphism $Z \in \mathbb{H}$ one verifies that $Z \circ (X \star Y) = (Z \circ X) \star (Z \circ Y)$. For a coalgebra homomorphism $Z \in \mathbb{H}$ we have $(X \star Y) \circ Z = (X \circ Z) \star (Y \circ Z)$.

As the shuffle product is commutative, one can show that if $X, Y \in \mathbb{H}$ are algebra homomorphisms, then $X \star Y$ is also an algebra homomorphism. The subset of algebra homomorphisms forms the group $\mathcal{H} \subset \mathbb{H}$ of $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ -valued characters, with unit ν . The inverse of $X \in \mathcal{H}$ is given by $X^{\star(-1)} := X \circ S$. Note \mathcal{H} is a subgroup of the Lie group

$$\mathcal{G} := \{X \in \mathbb{H}: X(\mathbf{1}) = \mathbf{1}\}.$$

The corresponding Lie algebra \mathfrak{h} of infinitesimal characters is a Lie subalgebra of the subalgebra

$$\mathfrak{g} := \{X \in \mathbb{H}: X(\mathbf{1}) = 0\},$$

of \mathbb{H} . The inverse in \mathcal{G} is given by $X^{\star(-1)} := \sum_{k \geq 0} (\nu - X)^{\star k}$. Note that we denote by $X^{\star k}$ the k -factor convolution product $X \star X \star \dots \star X$ for any $X \in \mathbb{H}$. Observe that, for $X \in \mathfrak{g}$, if w has length less than k then $X^{\star k} \circ w$ returns 0. Hence the formal sum for $X^{\star(-1)}$ makes sense and indeed, note that $(\nu - X) \in \mathfrak{g}$ for $X \in \mathcal{G}$. In fact we observe that $\mathcal{G} = \{\nu\} \oplus \mathfrak{g}$. See Manchon (2008), Patras & Reutenauer 2002 and Patras (1994) for more details.

An important endomorphism is the *augmented ideal projector* given by

$$J := \text{id} - \nu.$$

Thus J sends non-empty words to themselves, but the empty word to 0, i.e. $J \in \mathfrak{g}$. Note for example, $J^{\star k}$ takes a word w with $|w| \geq k$ and creates a sum of all possible k -partitions of w shuffled together (with the empty word an excluded partition). On the other hand, $\text{id}^{\star k}$ also includes all partitions involving the empty word. Now observe that the endomorphism F corresponding to the function f of the flowmap

above, with the power series coefficients $\{c_k\}$, is the endomorphism defined by the series in \mathbb{H} :

$$f^*(\text{id}) = \sum_{k=0}^{\infty} c_k \text{id}^{*k}.$$

More generally, we can consider functions on \mathbb{H} . For example, for $X \in \mathbb{H}$, with $X(\mathbf{1}) = \epsilon \mathbf{1}$ and $\epsilon \in \mathbb{K}$, we can construct an endomorphism through a series expansion about a multiple ϵ of the unit ν as follows:

$$f^*(X) = \sum_{k=0}^{\infty} c_k (X - \epsilon \nu)^{*k},$$

where $X - \epsilon \nu \in \mathfrak{g}$. Of particular interest are the bijective logarithm $\log^* : \mathcal{G} \rightarrow \mathfrak{g}$ and exponential $\exp^* : \mathfrak{g} \rightarrow \mathcal{G}$ maps defined for any $X \in \mathfrak{g}$ by

$$\log^*(\nu + X) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} X^{*k} \quad \text{and} \quad \exp^*(X) = \sum_{k=0}^{\infty} \frac{1}{k!} X^{*k}.$$

The sinhlog and coshlog maps are defined for $X \in \mathcal{G}$ by

$$\sinhlog^*(X) = \frac{1}{2}(X - X^{*(-1)}) \quad \text{and} \quad \coshlog^*(X) = \frac{1}{2}(X + X^{*(-1)}),$$

also have series representations in powers of $(X - \nu)$. These maps and their compositional inverses underlie our main result. For all $X, Y \in \mathbb{H}$, set h^* to be

$$h^*(X, Y) := (X^{*2} + Y)^{*(1/2)},$$

for which the square root exists. Then we have the compositional inverses

$$\sinhlog^{-1}(X) = X + h^*(X, +\nu) \quad \text{and} \quad \coshlog^{-1}(X) = X + h^*(X, -\nu),$$

i.e. we have $\sinhlog^{-1} \circ \sinhlog^*(X) = X$ and $\coshlog^{-1} \circ \coshlog^*(X) = X$.

To illustrate this new perspective and its natural connection to stochastic expansions, consider three examples. First, we observe that the stochastic Taylor expansion for the flowmap is simply the identity $\text{id} \in \mathcal{H}$. Second, the sinhlog function considered by Malham & Wiese (2009) is given by

$$\sinhlog^*(\text{id}) = \frac{1}{2}(\text{id} - S),$$

since $S = \text{id}^{*(-1)}$. In other words, applying the sinhlog function to the flowmap φ in $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \otimes \mathbb{K}\langle\mathbb{A}\rangle_{\text{co}}$, corresponds to applying \sinhlog^* to the identity $\text{id} \in \mathcal{H}$. Third, the Eulerian idempotent, which is a Lie idempotent from the free associative algebra to the free Lie algebra, is given by

$$\log^*(\text{id}) = J - \frac{1}{2}J^{*2} + \frac{1}{3}J^{*3} - \dots + \frac{(-1)^{k+1}}{k} J^{*k} + \dots.$$

This is the exponential Lie series or Chen–Strichartz formula (see Burgunder 2009, Chen 1957, Magnus 1954, Strichartz 1987 and Baudoin 2004). To see this we use that J^{*k} can be expressed as a sum over permutations with a prescribed descent set; see Reutenauer (1993; p. 65). Note also that since the antipode is the inverse of the identity with respect to the convolution product, then

$$S = \nu - J + J^{*2} - J^{*3} + \dots.$$

Hence we can also express the sinhlog endomorphism as

$$\text{sinhlog}^*(\text{id}) = J - \frac{1}{2}J^{*2} + \frac{1}{2}J^{*3} - \cdots + (-1)^{k+1}\frac{1}{2}J^{*k} + \cdots.$$

These three examples belong to the subalgebra of endomorphisms generated by the unit ν and augmented ideal projector J .

Remark 4 Note that the sinhlog and coshlog endomorphisms are projectors as $\frac{1}{2}(\text{id} \pm S) \circ \frac{1}{2}(\text{id} \pm S) = \frac{1}{2}(\text{id} \pm S)$ and $\frac{1}{2}(\text{id} \pm S) \circ \frac{1}{2}(\text{id} \mp S) = 0$.

We conclude this section by defining some endomorphisms and their properties useful in our subsequent analysis.

Definition 1 (Reversing and sign endomorphisms) These endomorphisms in \mathbb{H} are defined for any word $w = a_1 \dots a_n \in \mathbb{A}^*$ as follows: (1) Reversing endomorphism: $|S|: w \mapsto a_n \dots a_1$; and (2) Sign endomorphism: $D: w \mapsto (-1)^n w$.

Note, for example, that $D \circ D \equiv \text{id}$ and $S = D \circ |S| = |S| \circ D$. Observe also that since $S \in \mathcal{H}$ we have $|S|(u \sqcup v) = |S|(u) \sqcup |S|(v)$.

3 Convolution shuffle algebra with expectation inner product

We have seen that classes of endomorphisms $F \in \mathbb{H}$ correspond to functions of the flowmap. Our goal here is to define an appropriate inner product on \mathbb{H} and analyze its properties. This will be modelled on the mean-square measure of an \mathbb{R}^N -valued stochastic process, constructed as follows (hereafter the real parameter $t > 0$ is fixed).

3.1 Expectation endomorphism

Let $\mathbb{D}^* \subset \mathbb{A}^*$ denote the free monoid of words on the alphabet $\mathbb{D} = \{0, 11, \dots, dd\}$.

Definition 2 (Expectation map and endomorphism) The *expectation map* is the linear map $\bar{E}: \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \rightarrow \mathbb{K}$ which, in the case \mathbb{A} indexes d independent Wiener processes, is given by

$$\bar{E}: w \mapsto \begin{cases} t^{n(w)} / (2^{d(w)} n(w)!) & w \in \mathbb{D}^*, \\ 0 & w \in \mathbb{A}^* \setminus \mathbb{D}^*. \end{cases}$$

Here $d(w)$ is the number of non-zero consecutive pairs in w from the alphabet \mathbb{D} and $n(w) = z(w) + d(w)$, where $z(w)$ counts the number of '0' letters w contains.

We define the *expectation endomorphism* $E \in \mathbb{H}$ as

$$E: w \mapsto \bar{E}(w) \mathbf{1}.$$

Note the endomorphisms $X - E \circ X \equiv (\text{id} - E) \circ X$ in \mathbb{H} have zero expectation. Indeed $(\text{id} - E)$ lies in the kernel of E as $E \circ E = E$.

Remark 5 Strictly, the expectation map $\bar{E}: \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \rightarrow \mathbb{K}[t]$, where t is a parameter commuting with all of $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$, and $(\text{id} - E) \circ X$ takes values in $\mathbb{K}[t] \mathbf{1} \oplus \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$.

Remark 6 The values quoted for the expectation map for any $w \in \mathbb{A}^*$ are the expectations of the corresponding multiple Stratonovich integrals, see Kloeden & Platen (1999; eqns (5.2.34), (5.7.1)) or Buckwar *et al.* (2012). Briefly, every Stratonovich integral labelled by $w \in \mathbb{A}^*$, is a linear combination of Itô integrals. The Itô integrals concerned, cycle through the set of words which consist of w and all words u obtained by successively replacing any two adjacent non-zero equal indices in w by 0. Each replacement contributes a factor one-half to the coefficient of the Itô integral in the linear combination. Since the expectation of any Itô integral is zero unless all its labelling letters are 0, the expectation of the Stratonovich integral is given by the deterministic integral remaining after the replacement process (and zero if there isn't one).

3.2 Inner product of endomorphisms

Let $\{V_w\}_{w \in \mathbb{A}^*}$ denote a given set of indeterminate vectors indexed by words $w \in \mathbb{A}^*$. We use both (u, v) and V_{uv} to denote the inner product of the vectors V_u and V_v . Let V denote the infinite square matrix indexed by the words $u, v \in \mathbb{A}^*$ with entries $V_{u,v}$.

Definition 3 (Inner product) We define the *inner product* of $X, Y \in \mathbb{H}$ with respect to V to be

$$\langle X, Y \rangle_{\mathbb{H}} := \sum_{u, v \in \mathbb{A}^*} \bar{E}(X(u) \sqcup Y(v))(u, v).$$

The norm of an endomorphism $X \in \mathbb{H}$ is $\|X\|_{\mathbb{H}} := \langle X, X \rangle^{1/2}$.

Let us motivate this definition and provide some equivalent characterizations. Suppose we apply two separate functions to the flowmap φ which are characterized by the endomorphisms X and Y in \mathbb{H} . We assume the governing vector fields and driving Wiener processes are given as well as some data $y_0 \in \mathbb{R}^N$. With a slight abuse of notation we express the two stochastic processes x_t and y_t associated with X and Y as follows

$$x_t = \sum_{w \in \mathbb{A}^*} X(w) V_w(y_0) \quad \text{and} \quad y_t = \sum_{w \in \mathbb{A}^*} Y(w) V_w(y_0).$$

Our definition is based on the L^2 -inner product $\langle x_t, y_t \rangle_{L^2} = \bar{E}(x_t, y_t)$. We would like our inner product to be independent of the data y_0 , hence we replace the vector fields evaluated at the data by the set of indeterminants $\{V_w\}_{w \in \mathbb{A}^*}$.

An equivalent characterization of the inner product is as follows. The action of an endomorphism X on a word can be written $X(w) = \sum_{u \in \mathbb{A}^*} X_{w,u} u$, for some \mathbb{K} -valued coefficients $X_{w,u}$. In other words we can represent $X \in \mathbb{H}$ by a matrix $X \in \mathbb{K}^\infty \times \mathbb{K}^\infty$ indexed by the words $w \in \mathbb{A}^*$. We can order the indexing by word length and then lexicographically within each length (for example). Now let $W \in \mathbb{K}^\infty \times \mathbb{K}^\infty$ denote the symmetric matrix of values $\bar{E}\{u \sqcup v\}$ over all $u, v \in \mathbb{A}^*$ and $V \in \mathbb{K}^\infty \times \mathbb{K}^\infty$ the symmetric matrix defined above. Then using our definition

above, we observe that

$$\begin{aligned}\langle X, Y \rangle_{\mathbb{H}} &= \sum_{u, v, u', v' \in \mathbb{A}^*} \mathbf{X}_{u, u'} \mathbf{Y}_{v, v'} \mathbf{W}_{u', v'} \mathbf{V}_{u, v} \\ &= \text{tr}(\mathbf{X} \mathbf{W} \mathbf{Y}^\dagger \mathbf{V}^\dagger) \\ &= \text{tr}(\mathbf{V}^{\frac{1}{2}} \mathbf{X} \mathbf{W} \mathbf{Y}^\dagger (\mathbf{V}^{\frac{1}{2}})^\dagger),\end{aligned}$$

where \dagger denotes matrix transpose. Note that both \mathbf{W} and \mathbf{V} are positive definite. Hence we can view the definition of the inner product above as defined with respect to the weights \mathbf{W} and \mathbf{V} where the stochastic and geometric information are respectively encoded. All results we subsequently establish will hold independent of \mathbf{V} . Lastly, we now note that our inner product is: (i) Symmetric as the shuffle product and vector inner product are commutative; (ii) Bilinear as the endomorphisms and expectation are linear; (iii) Positive definite as the matrix of expectations \mathbf{W} is positive definite.

Remark 7 We assume that the solution to our stochastic differential system for any data y_0 is L^2 -valued on the time interval of interest. This is equivalent to saying that $\|\text{id}\|_{\mathbb{H}}^2$ is finite, which is equivalent to assuming $\text{tr}(\mathbf{W}\mathbf{V})$ is finite.

3.3 Graded class subspace

We often will be concerned with endomorphisms that act on subspaces of $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ selected according to a grading. Recall that $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ is a connected Hopf algebra graded by the length of words.

Definition 4 (Grading map) This is the linear map $g: \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \rightarrow \mathbb{Z}_+$ given by

$$g: w \mapsto |w|.$$

The empty word has length zero, i.e. $|\mathbf{1}| = 0$.

Remark 8 There is another natural grading on \mathbb{A}^* given by the variance of the words $w \in \mathbb{A}^*$, as mentioned in the introduction. This is determined by the exponent in t when computing the root-mean-square deviation from the expectation of w , i.e. the square-root of $\bar{E} \circ (w - E(w))^{\perp\perp}$. Briefly, for any word w , zero letters contribute a count of one while non-zero letters contribute a count of one-half towards the grade value. The nuances of the two gradings are revealed in §5.

Definition 5 (Graded class subspace) For a given $n \in \mathbb{Z}_+$, let \mathbb{S}_n denote the subspace of $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ of all words w of given length $g(w) = n$. We set

$$\mathbb{S}_{\leq n} := \bigoplus_{k \leq n} \mathbb{S}_k \quad \text{and} \quad \mathbb{S}_{\geq n} := \bigoplus_{k \geq n} \mathbb{S}_k.$$

A subspace \mathbb{S} is a *graded class subspace* if, for a given $n \in \mathbb{Z}_+$, $\mathbb{S} = \mathbb{S}_n$, $\mathbb{S} = \mathbb{S}_{\leq n}$ or $\mathbb{S} = \mathbb{S}_{\geq n}$. For any graded class subspace \mathbb{S} , we denote by

$$\pi_{\mathbb{S}}: \mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}} \rightarrow \mathbb{S},$$

the canonical projection from $\mathbb{K}\langle\mathbb{A}\rangle_{\text{sh}}$ onto \mathbb{S} .

Hereafter we set, for any graded class subspace \mathbb{S} , for all $X, Y \in \mathbb{H}$:

$$\langle X, Y \rangle := \langle X \circ \pi_{\mathbb{S}}, Y \circ \pi_{\mathbb{S}} \rangle_{\mathbb{H}} \quad \text{and} \quad \|X\| := \|X \circ \pi_{\mathbb{S}}\|_{\mathbb{H}}.$$

We carefully state the subspace \mathbb{S} in all instances, so no confusion should arise.

3.4 Properties of the sinhlog and coshlog endomorphisms

The following lemma from Malham & Wiese (2009) is a crucial ingredient in what follows. We restate it here and discuss an extension we rely upon for clarity.

Lemma 1 (Malham & Wiese (2009); Lemma 4.3) *For any pair $u, v \in \mathbb{A}^*$, we have $E(u \sqcup v) \equiv E(|S| \circ u) \sqcup (|S| \circ v)$.*

Though the context for this lemma was the alphabet $\mathbb{A} = \{1, \dots, d\}$, it in fact extends to $\mathbb{A} = \{0, 1, \dots, d\}$. The proof detailed in Malham & Wiese relies on two results. First, any Stratonovich integral can be expressed as a linear combination of Itô integrals, as described in Remark 6 (also see Kloeden & Platen 1999; eqn (5.2.34)). Importantly, reversing the word associated with a Stratonovich integral generates a mirror linear combination of Itô integrals with their respective words reversed (with the same coefficients). Second, the expectation of the product of any two Itô integrals only depends on the number of non-zero letters and the lengths of subwords containing only 0 letters. These characteristic quantities are invariant to reversing the words concerned (see Kloeden & Platen 1999; Lemma 5.7.2). Both of these results from Kloeden & Platen are stated for $\mathbb{A} = \{0, 1, \dots, d\}$.

Remark 9 Importantly, note that if u and v have the same length, then we can replace $|S|$ by S as the result is then invariant to the sign in the antipode S . This observation underlies the restriction to $\mathbb{S} = \mathbb{S}_n$ when $\mathbb{A} = \{0, 1, \dots, d\}$ in Lemma 2 below.

We now state the main lemma of this section, outlining properties of the principle endomorphisms we have thusfar highlighted, in particular the endomorphisms

$$\text{sinhlog}^*(\text{id}) = \frac{1}{2}(\text{id} - S) \quad \text{and} \quad \text{coshlog}^*(\text{id}) = \frac{1}{2}(\text{id} + S).$$

The results herein are used to establish the optimal efficiency properties of the sinhlog integrator in §4.

Lemma 2 *We assume either, $\mathbb{A} = \{0, 1, \dots, d\}$ and \mathbb{S} is the graded class subspace $\mathbb{S} = \mathbb{S}_n$, or, $\mathbb{A} = \{1, \dots, d\}$ and \mathbb{S} is any graded class subspace. Then for any $X, Y \in \mathbb{H}$ (and for any \mathbb{V}) we have the following properties:*

1. $\langle X, Y \rangle = \langle |S| \circ X, |S| \circ Y \rangle$;
2. $\langle |S|, |S| \rangle = \langle S, S \rangle = \langle \text{id}, \text{id} \rangle$;
3. $\langle \text{sinhlog}^*(\text{id}), \text{coshlog}^*(\text{id}) \rangle = 0$;
4. $\|\text{id}\|^2 = \|\text{sinhlog}^*(\text{id})\|^2 + \|\text{coshlog}^*(\text{id})\|^2$;
5. $\langle X, E \circ Y \rangle = \langle E \circ X, E \circ Y \rangle$;
6. $\langle E \circ \text{id}, E \circ \text{id} \rangle = \langle E \circ |S|, E \circ |S| \rangle = \langle E \circ S, E \circ S \rangle$;
7. $\langle E \circ \text{sinhlog}^*(\text{id}), E \circ \text{coshlog}^*(\text{id}) \rangle = 0$;
8. $\langle |S|, J^{*n} \rangle = \langle \text{id}, J^{*n} \rangle$,

where property 8 only holds for $\mathbb{S} = \mathbb{S}_n$, independent of the alphabet. Property 3 indicates $\text{sinhlog}^*(\text{id})$ and $\text{coshlog}^*(\text{id})$ are orthogonal with respect to the inner product.

Proof We establish properties 1–8 in order. Using the linearity properties of the expectation map and reversing endomorphism $|S|$ we observe that

$$\begin{aligned} E(X(u) \sqcup Y(v)) &= \sum_{w_1, w_2} X_{uw_1} Y_{vw_2} E(w_1 \sqcup w_2) \\ &= \sum_{w_1, w_2} X_{uw_1} Y_{vw_2} E((|S| \circ w_1) \sqcup (|S| \circ w_2)) \\ &= E((|S| \circ X)(u) \sqcup (|S| \circ Y)(v)), \end{aligned}$$

and property 1 follows. Property 2 is a special case of property 1. Using property 2 and Lemma 1 we deduce that $4\langle \text{sinhlog}^*(\text{id}), \text{coshlog}^*(\text{id}) \rangle = \langle \text{id}, \text{id} \rangle - \langle S, S \rangle = 0$, thus establishing property 3. Property 4 follows directly when we observe that sinhlog and coshlog additively decompose the identity, i.e. $\text{id} = \text{sinhlog}^*(\text{id}) + \text{coshlog}^*(\text{id})$. Properties 5–7 now follow from the properties of the expectation endomorphism. Property 8 follows directly from the commutativity of the shuffle product.

4 Sinhlog and the optimal efficient integrator

Recall our construction of a stochastic integrator for a given smooth function $f: \text{Diff}(\mathbb{R}^N) \rightarrow \text{Diff}(\mathbb{R}^N)$ we outlined in steps 1–3 in the introduction. In terms of the convolution shuffle algebra and corresponding endomorphism $f^*(\text{id}) \in \mathbb{H}$, those steps and concepts therein, have natural concise translations. Proceeding through the construction, by direct analogy with $\hat{\varphi}_t$, a general stochastic integrator has the form

$$\hat{\text{id}} := f^{-1} \circ \pi_{\mathbb{S}_{\leq n}} \circ f^*(\text{id}).$$

The error associated with this approximation is

$$R := \text{id} - \hat{\text{id}}.$$

One integrator will be more accurate than another if the \mathbb{H} -norm of its associated error $\|R\|_{\mathbb{H}}$ is smaller than the other.

Remark 10 In light of our comments in the introduction that the set of Lyndon word multiple integrals included in an integrator determine its order, we will restrict ourselves to functions $f^*: \mathbb{H} \rightarrow \mathbb{H}$ that are grade preserving. All the functions herein such as the logarithm, exponential, sinhlog, coshlog or any power series in J are grade preserving (their action on words generates linear combinations of words of the same length).

Remark 11 Also as mentioned in the introduction, we need to include the expectations of the terms in the remainder in \mathbb{S}_{n+1} in the integrator. These are in general encoded by $E \circ \pi_{\mathbb{S}_{n+1}} \circ R$, so the effective *leading order terms* in the remainder are $(\text{id} - E) \circ \pi_{\mathbb{S}_{n+1}} \circ R$. We highlight this at the appropriate junctures.

Definition 6 (Pre-remainder) We define the *pre-remainder* Q to be the remainder terms after applying the endomorphism $f^*(\text{id})$ and then truncating to include the terms in $\mathbb{S}_{\leq n}$, i.e. it is

$$Q := f^*(\text{id}) - \pi_{\mathbb{S}_{\leq n}} \circ f^*(\text{id}).$$

The relationship between R and Q plays a key role in our subsequent analysis.

We now examine the properties of integrators based on the sinhlog endomorphism, indeed of a whole class of endomorphisms to which it belongs, as well as the coshlog endomorphism. First we focus on the sinhlog endomorphism and re-establish that it is an efficient integrator, in the context of the convolution shuffle algebra. As we do so, we will see natural questions that emerge, motivating us to dig deeper.

Definition 7 (Efficient integrator) A numerical approximation to the solution of a stochastic differential equation is an *efficient integrator* if it generates a strong numerical integration scheme that is more accurate in the mean square sense than the corresponding stochastic Taylor integration scheme of the same strong order, independent of the governing vector fields and to all orders. In other words, if R denotes the remainder of an integrator, it is efficient if for $\mathbb{S} = \mathbb{S}_{n+1}$ for any n , and for any \mathbb{V} :

$$\|(\text{id} - E) \circ R\|^2 \leq \|(\text{id} - E) \circ \text{id}\|^2.$$

The sinhlog endomorphism of interest has the expansion

$$\text{sinhlog}^*(\text{id}) = J - \frac{1}{2}J^{*2} + \frac{1}{2}J^{*3} - \frac{1}{2}J^{*4} + \dots$$

To construct a sinhlog integrator of strong order $n/2$, we start by applying the projection operator $\pi_{\mathbb{S}_{\leq n}}$ to $\text{sinhlog}^*(\text{id})$; call the result

$$P := \pi_{\mathbb{S}_{\leq n}} \circ \text{sinhlog}^*(\text{id}).$$

Since $J^{*(n+1)}$ is zero for any words w with $|w| < n+1$ and each of the terms in the expansion above is grade preserving, we see that

$$P = \left(J - \frac{1}{2}J^{*2} + \dots + \frac{1}{2}(-1)^{n+1}J^{*n} \right) \circ \pi_{\mathbb{S}_{\leq n}}.$$

The pre-remainder is thus given by

$$Q = \text{sinhlog}^*(\text{id}) \circ \pi_{\mathbb{S}_{\geq n+1}}.$$

The compositional inverse of the sinhlog endomorphism is given by $\text{sinhlog}^{-1} \circ X = X + h^*(X, +\nu)$ where $h^*(X, +\nu) := (\nu + X^{*2})^{*(1/2)}$ has the expansion

$$h^*(X, +\nu) = \nu + \frac{1}{2}X^{*2} - \frac{1}{8}X^{*4} + \dots$$

By definition, the error R in the approximation $\text{id} = \text{sinhlog}^{-1} \circ P$ is given by

$$\begin{aligned} R &= \text{id} - \text{sinhlog}^{-1} \circ P \\ &= \text{sinhlog}^{-1} \circ (P + Q) - \text{sinhlog}^{-1} \circ P \\ &= Q + h^*(P + Q, +\nu) - h^*(P, +\nu) \\ &= Q + \frac{1}{2}((P + Q)^{*2} - P^{*2}) + \dots \end{aligned}$$

$$= Q + \frac{1}{2}(P \star Q + Q \star P) + \mathcal{O}(Q^{\star 2}).$$

The leading order term in R is

$$Q \circ \pi_{\mathbb{S}_{n+1}}.$$

We justify this as follows. Consider the term $P \star Q$. Since at leading order $\text{sinhlog}^*(\text{id}) = J$, we see at leading order

$$P \star Q = (J \circ \pi_{\mathbb{S}_{\leq n}}) \star (J \circ \pi_{\mathbb{S}_{\geq n+1}}).$$

This means that for some coefficients $c_w \in \mathbb{K}$,

$$\sum_w ((P \star Q) \circ w) \otimes w = \sum_{|w| \geq n+2} c_w w \otimes w.$$

This follows from the fact that the two indicator functions annihilate any lower order terms in the two-part deconcatenation implied by the convolution, and that J annihilates the empty word. We also only retain the leading order terms in Q by applying $\pi_{\mathbb{S}_{n+1}}$ as shown in the final step above.

Remark 12 We shall use the big \mathcal{O} notation such as $\mathcal{O}(P \star Q)$ or $\mathcal{O}(Q^{\star 2})$ above to denote endomorphisms that only generate terms involving words that are higher order with respect to the grading g than those generated by the preceding endomorphisms.

Thus using Lemma 2(3) with $\mathbb{S} = \mathbb{S}_{n+1}$ we have

$$\|\text{id}\|^2 = \|Q\|^2 + \|\text{coshlog}^*(\text{id})\|^2.$$

Now using $\text{id} = \text{sinhlog}^*(\text{id}) + \text{coshlog}^*(\text{id})$ and Lemma 2(5,7) we deduce that

$$\|(\text{id} - E) \circ \text{id}\|^2 = \|(\text{id} - E) \circ Q\|^2 + \|(\text{id} - E) \circ \text{coshlog}^*(\text{id})\|^2.$$

Recall from Remark 11 that we need to include in our integrators the expectation of the leading order terms in the remainder. This means the remainders for the stochastic Taylor expansion and sinhlog integrators are $(\text{id} - E \circ \text{id}) \circ \pi_{\mathbb{S}_{n+1}}$ and $(Q - E \circ Q) \circ \pi_{\mathbb{S}_{n+1}}$, respectively, since at leading order $R = Q \circ \pi_{\mathbb{S}_{n+1}}$. We have thus established that integrators based on the sinhlog endomorphism are at least as accurate as corresponding stochastic Taylor integrators at leading order, i.e. they are efficient.

We can prove the following extension of Corollary 4.2 in Malham & Wiese (2009) to the alphabet $\mathbb{A}^* = \{0, 1, \dots, d\}$; indeed assume this to be the alphabet hereafter.

Lemma 3 *With $\mathbb{S} = \mathbb{S}_{n+1}$, if n is odd, then the error of the sinhlog integrator is optimal; it realizes its smallest possible value compared to the error of the corresponding stochastic Taylor integrator.*

Proof To prove this, order by order we perturb the sinhlog integrator as follows. For a fixed $n \in \mathbb{N}$ perturb the coefficient of $J^{*(n+1)}$ in the sinhlog expansion so that

$$\text{sinhlog}_\epsilon^*(\text{id}) = J + \frac{1}{2} \sum_{k=2}^{\infty} (-1)^{k+1} J^{*k} + \epsilon J^{*(n+1)},$$

where $\epsilon \in \mathbb{R}$ is a parameter. Then repeating the procedure above, we have

$$Q_\epsilon = (\text{sinhlog}_\epsilon^*(\text{id}) + \epsilon J^{*(n+1)}) \circ \pi_{\mathbb{S}_{\geq n+1}}.$$

Since the leading order behaviour of the inverse of sinhlog^* is unaffected, we have at leading order $R_\epsilon = Q_\epsilon$. As above, truncate Q_ϵ with $\pi_{\mathbb{S}_{n+1}}$. Then with $\mathbb{S} = \mathbb{S}_{n+1}$ we see

$$\begin{aligned} \|\text{id}\|^2 &= \langle Q_\epsilon + \text{coshlog}^*(\text{id}) - \epsilon J^{*(n+1)}, Q_\epsilon + \text{coshlog}^*(\text{id}) - \epsilon J^{*(n+1)} \rangle \\ &= \|Q_\epsilon\|^2 + 2\langle Q_\epsilon, \text{coshlog}^*(\text{id}) - \epsilon J^{*(n+1)} \rangle + \|\text{coshlog}^*(\text{id}) - \epsilon J^{*(n+1)}\|^2 \\ &= \|Q_\epsilon\|^2 + \|\text{coshlog}^*(\text{id})\|^2 - 2\epsilon \langle \text{sinhlog}^*(\text{id}), J^{*(n+1)} \rangle - \epsilon^2 \|J^{*(n+1)}\|^2 \\ &= \|Q_\epsilon\|^2 + \|\text{coshlog}^*(\text{id})\|^2 - \epsilon \langle \text{id} - S, J^{*(n+1)} \rangle - \epsilon^2 \|J^{*(n+1)}\|^2, \end{aligned}$$

where in the penultimate step we used the orthogonality property of sinhlog and coshlog. When we include the expectations of the leading order terms in the remainder (cf. Remark 11) this relation becomes

$$\begin{aligned} \|(\text{id} - E) \circ \text{id}\|^2 &= \|(\text{id} - E) \circ Q_\epsilon\|^2 + \|(\text{id} - E) \circ \text{coshlog}^*(\text{id})\|^2 \\ &\quad - \epsilon \langle (\text{id} - E) \circ (\text{id} - S), (\text{id} - E) \circ J^{*(n+1)} \rangle \\ &\quad - \epsilon^2 \|(\text{id} - E) \circ J^{*(n+1)}\|^2. \end{aligned}$$

The linear term in ϵ is zero if n is odd, by Lemma 2(8). Hence in this case, the mean-square excess, the terms on the right other than $\|Q_\epsilon\|^2$, is optimized when $\epsilon = 0$.

Remark 13 This result can be found in Malham & Wiese (2009) for $\mathbb{A} = \{1, \dots, d\}$. It extends to $\mathbb{A} = \{0, 1, \dots, d\}$ using Lemma 2, though under the proviso that we grade according to word length. This means that we endeavour to include some multiple integrals in our stochastic integrator involving the drift ‘0’ index that we would not ordinarily include if we were grading according to variance (of the multiple Wiener integrals). However we take the perspective here that there are far fewer of these terms at each grading according to length, and the computational effort associated with their simulation is a small fraction of that overall. If we include them, we guarantee efficiency. See §5 for an example. Of course if $\mathbb{A} = \{1, \dots, d\}$ only, then the two notions of grading coincide and this technicality is redundant.

Some natural questions now arise. It is apparent that the first key result in the argument above to prove efficiency was Lemma 2(4) showing that the norm-square of the identity endomorphism decomposes into the sum of the norm-squares of the sinhlog and coshlog endomorphisms. The second key result, to prove that the sinhlog integrator was optimal when n is odd, was Lemma 2(8). First, with regard to efficiency and Lemma 2(4). Since there is no immediate apparent difference, it

would seem we could choose coshlog as our integrator endomorphism. Further, the result of Lemma 2(4) essentially relied on the fact that $\langle S, S \rangle = \langle \text{id}, \text{id} \rangle$. However, we also know from Lemma 2(2) that $\langle |S|, |S| \rangle = \langle \text{id}, \text{id} \rangle$. Thus, in principle, we could also consider $\frac{1}{2}(\text{id} - |S|)$ as an integrator (or indeed any pair $\frac{1}{2}(\text{id} \pm X)$ for which $\langle X, X \rangle = \langle \text{id}, \text{id} \rangle$). Note that $\frac{1}{2}(\text{id} - |S|)$ is the equivalent of applying the sinhlog endomorphism at even orders and the coshlog endomorphism at odd orders. Second, with regard to optimal efficiency, it would also seem that $\frac{1}{2}(\text{id} - |S|)$ would deliver optimality at both even and odd orders as the linear term in ϵ above would be zero. However, this is not the case. The key is the relation between the error R and the pre-remainder Q .

We define the following class of endomorphisms, set

$$f^*(X; \epsilon) := \frac{1}{2}(X - \epsilon X^{*(-1)}).$$

for any $\epsilon \in \mathbb{R}$. Then we see $f^*(\text{id}, +1)$ is the sinhlog endomorphism and $f^*(\text{id}, -1)$ is the coshlog endomorphism. Note that the compositional inverse of $f^*(X; \epsilon)$ is

$$f^{-1}(X; \epsilon) = X + h^*(X, \epsilon \nu),$$

where $h^* = h^*(X, Y)$ is the convolutional square root of $X^{*2} + Y$ given in the introduction. Our main result is as follows.

Theorem 1 *For every $\epsilon > 0$ the class of integrators $f^*(\text{id}; \epsilon)$ is efficient. When $\epsilon = 1$, the error of the integrator $f^*(\text{id}; 1)$ realizes its smallest possible value compared to the error of the corresponding stochastic Taylor integrator, i.e. if R_ϵ denotes the remainder of the integrator, we have that the mean-square excess*

$$\|(\text{id} - E) \circ \text{id}\|^2 - \|(\text{id} - E) \circ R_\epsilon\|^2$$

is positive and maximized at $\epsilon = 1$. Thus a strong stochastic integrator based on the sinhlog endomorphism is optimally efficient within this class.

Proof We prove the theorem in four steps. Note that we have for any $\epsilon \in \mathbb{R}$:

$$f^*(\text{id}; \epsilon) = \frac{1}{2}(1 - \epsilon)\nu + \frac{1}{2}(1 + \epsilon)J - \frac{1}{2}\epsilon(J^{*2} - J^{*3} + \dots).$$

The integrator of interest of strong order $n/2$ is $P := \pi_{\mathbb{S}_{\leq n}} \circ f^*(\text{id}; \epsilon)$ and given by

$$P = \left(\frac{1}{2}(1 - \epsilon)\nu + \frac{1}{2}(1 + \epsilon)J - \frac{1}{2}\epsilon(J^{*2} - J^{*3} + \dots + (-1)^n J^{*n}) \right) \circ \pi_{\mathbb{S}_{\leq n}}.$$

The pre-remainder is $Q = f^*(\text{id}; \epsilon) \circ \pi_{\mathbb{S}_{\geq n+1}}$. Further, the approximation $\hat{\text{id}} := f^{-1} \circ P$ results in an error given by

$$\begin{aligned} R &= \text{id} - \hat{\text{id}} \\ &= f^{-1} \circ (P + Q) - f^{-1} \circ P \\ &= Q + h^*(P + Q, \epsilon \nu) - h^*(P, \epsilon \nu). \end{aligned}$$

Our goal now is to carefully examine this relationship between R and Q , and in particular, the difference on the right shown.

Step 1. A thorough understanding of the function h^* is thus required, and we motivate our analysis by considering the corresponding real-valued function $h: \mathbb{R}^2 \rightarrow \mathbb{R}$ given by

$$h: (x, y) \mapsto (x^2 + y)^{1/2}.$$

The function $h = h(x, y)$ is real-analytic for $y > -x^2$, zero on $y = -x^2$ where its tangent plane is orthogonal to the (x, y) -plane, and complex-valued elsewhere. Hence we can choose a point inside the open region $y > -x^2$ about which the Taylor series for $h = h(x, y)$ has a non-zero radius of convergence. In particular for $y > -x^2$, the difference $h(x + q, y) - h(x, y)$ at leading order in q is given by

$$h(x + q, y) - h(x, y) = \frac{x}{(x^2 + y)^{1/2}} \cdot q + \dots$$

Step 2. By analogy with Step 1 we see in the convolution algebra we can expand

$$\begin{aligned} R &= Q + h^*(P + Q, \epsilon \nu) - h^*(P, \epsilon \nu) \\ &= Q + ((P + Q)^{\star 2} + \epsilon \nu)^{\star(1/2)} - (P^{\star 2} + \epsilon \nu)^{\star(1/2)} \\ &= Q + (P^{\star 2} + \epsilon \nu)^{\star(1/2)} \\ &\quad \star \left(\left(\nu + (P^{\star 2} + \epsilon \nu)^{\star(-1)} \star (P \star Q + Q \star P + Q^{\star 2}) \right)^{\star(1/2)} - \nu \right) \\ &= Q + \frac{1}{2}(P^{\star 2} + \epsilon \nu)^{\star(-1/2)} \star \left((P \star Q + Q \star P) + \mathcal{O}(Q^{\star 2}) \right). \end{aligned}$$

Further we note that at leading order

$$P = \frac{1}{2}(1 - \epsilon) \nu + \frac{1}{2}(1 + \epsilon) J + \mathcal{O}(J^{\star 2}),$$

and thus for all $\epsilon > -1$ we have

$$(P^{\star 2} + \epsilon \nu)^{\star(-1/2)} = \left(\frac{1}{2}(1 + \epsilon) \right)^{-1} \nu + \mathcal{O}(J).$$

Substituting these expressions into that for R above, we get at leading order:

$$\begin{aligned} R &= Q + \frac{1 - \epsilon}{1 + \epsilon} Q + \mathcal{O}(J \star Q) \\ &= \frac{2}{1 + \epsilon} Q \circ \pi_{\mathbb{S}_{n+1}}. \end{aligned}$$

Step 3. Let us now compare the mean-square error of P to the corresponding stochastic Taylor integrator $\text{id} \circ \pi_{\mathbb{S}_{\leq n}}$. We see that on \mathbb{S}_{n+1} we have

$$\begin{aligned} \|\text{id}\|^2 &= \langle R + \text{id} - R, R + \text{id} - R \rangle \\ &= \|R\|^2 + 2\langle R, \text{id} - R \rangle + \langle \text{id} - R, \text{id} - R \rangle \\ &= \|R\|^2 + 2 \left\langle \text{id} - \frac{1}{1 + \epsilon} (\text{id} - \epsilon S), \frac{1}{1 + \epsilon} (\text{id} - \epsilon S) \right\rangle \\ &\quad + \left\langle \text{id} - \frac{1}{1 + \epsilon} (\text{id} - \epsilon S), \text{id} - \frac{1}{1 + \epsilon} (\text{id} - \epsilon S) \right\rangle \end{aligned}$$

$$\begin{aligned}
&= \|R\|^2 + \|\text{id}\|^2 - \frac{1}{(1+\epsilon)^2} (\|\text{id}\|^2 - 2\epsilon \langle \text{id}, S \rangle + \epsilon^2 \|S\|^2) \\
&= \|R\|^2 + \frac{2\epsilon}{(1+\epsilon)^2} (\|\text{id}\|^2 + \langle \text{id}, S \rangle).
\end{aligned}$$

If we include the expectations of the leading order terms in the integrator (again cf. Remark 11) then we have

$$(\text{id} - E) \circ R = \frac{2}{1+\epsilon} (\text{id} - E) \circ Q \circ \pi_{\mathbb{S}_{n+1}}.$$

The comparison above becomes

$$\begin{aligned}
\|(\text{id} - E) \circ \text{id}\|^2 &= \|(\text{id} - E) \circ R\|^2 \\
&\quad + \frac{2\epsilon}{(1+\epsilon)^2} (\|(\text{id} - E) \circ \text{id}\|^2 + \langle (\text{id} - E) \circ \text{id}, (\text{id} - E) \circ S \rangle).
\end{aligned}$$

Step 4. We see the mean-square excess is

$$\frac{2\epsilon}{(1+\epsilon)^2} (\|(\text{id} - E) \circ \text{id}\|^2 + \langle (\text{id} - E) \circ \text{id}, (\text{id} - E) \circ S \rangle).$$

Note for any $X, Y \in \mathbb{H}$ we have $|\langle X, Y \rangle| \leq \|X\| \|Y\|$. Using Lemma 2 we see that

$$\begin{aligned}
\|(\text{id} - E) \circ |S|\|^2 &= \langle |S|, |S| \rangle - \langle E \circ |S|, E \circ |S| \rangle \\
&= \langle \text{id}, \text{id} \rangle - \langle E \circ \text{id}, E \circ \text{id} \rangle \\
&= \|(\text{id} - E) \circ \text{id}\|^2.
\end{aligned}$$

Hence we observe that $\langle (\text{id} - E) \circ \text{id}, (\text{id} - E) \circ |S| \rangle \leq \|(\text{id} - E) \circ \text{id}\|^2$, and thus

$$0 < \left| \langle (\text{id} - E) \circ \text{id}, (\text{id} - E) \circ S \rangle \right| \leq \|(\text{id} - E) \circ \text{id}\|^2.$$

Note all our statements above hold for any \mathbb{V} . Hence for all $\epsilon > 0$, the mean-square excess is positive and thus P is a uniformly accurate integrator, thus establishing the first statement of the theorem. When $\epsilon = 0$ the mean-square excess is zero as expected. For $\epsilon < 0$ it is negative. Further we see that for $\epsilon > 0$ the mean-square excess is largest when $\epsilon = 1$, corresponding to the sinhlog endomorphism. We have thus established the second statement of the theorem and the proof is complete.

Note when $\epsilon = -1$ the mean-square excess in Step 4 of the proof above is undefined. We can explain this as follows. The first equation in Step 2 becomes

$$R = Q + \frac{1}{2}(P^{\star 2} - \nu)^{\star(-1/2)} \star (P \star Q + Q \star P) + \mathcal{O}(Q^{\star 2}).$$

However now the leading order behaviour in P is $P = \nu + \frac{1}{2}J^{\star 2} + \mathcal{O}(J^{\star 3})$. If we denote $\hat{P} = P - \nu$ then we see that

$$\begin{aligned}
(P^{\star 2} - \nu)^{\star(1/2)} &= ((\nu + \hat{P})^{\star 2} - \nu)^{\star(1/2)} \\
&= \sqrt{2} \hat{P}^{\star(1/2)} \star (\nu + \frac{1}{2}\hat{P})^{\star(1/2)} \\
&= \sqrt{2} \hat{P}^{\star(1/2)} \star \left(\nu + \frac{1}{4}\hat{P} + \mathcal{O}(\hat{P}^{\star 2}) \right).
\end{aligned}$$

Proceeding formally, we substitute these last two expansions into the expression for R above. Retaining leading order terms we find

$$R = Q + (J^{*(-1)} \circ \pi_{\mathbb{S}_{\leq n}}) * Q + \mathcal{O}(J * Q).$$

In other words, the term in the error R corresponding to the difference of h^* evaluated at $P + Q$ and P generates the term $(J^{*(-1)} \circ \pi_{\mathbb{S}_{\leq n}}) * Q$. The inverse of J is not an element of the group \mathcal{G} . It does have the formal expansion $J^{*(-1)} = S + S^{*2} + S^{*3} + \dots$, but this does not have a finite evaluation on the empty word. Hence on \mathbb{S}_{n+1} , the term $(J^{*(-1)} \circ \pi_{\mathbb{S}_{\leq n}}) * Q$ is not finite. However it is finite on \mathbb{S}_n —the inverse contracts the number of deconcatenations—but this now introduces terms in the remainder of the same order as those we retain in the integrator, i.e. we have a form of order reduction.

5 Concluding remarks

We established the sinhlog integrator is optimally efficient when we grade according to word length. For example, the sinhlog integrator specified by $g(w) \leq 2$ on the computation interval $[t_n, t_{n+1}]$ is given by

$$y_{n+1} = \text{sinhlog}^{-1}(\hat{\sigma}_{n,n+1}) \circ y_n,$$

where

$$\hat{\sigma}_{n,n+1} = \sum_{i=0}^d J_i(t_n, t_{n+1}) V_i + \sum_{i,j=0}^d \frac{1}{2} (J_{ij} - J_{ji})(t_n, t_{n+1}) V_{ij}.$$

Whatever the vector fields are, this is guaranteed to be more accurate than

$$y_{n+1} = y_n + \sum_{i=0}^d J_i(t_n, t_{n+1}) V_i(y_n) + \sum_{i,j=0}^d J_{ij}(t_n, t_{n+1}) V_{ij}(y_n),$$

which is the corresponding integrator based on the stochastic Taylor expansion according to the grading $g(w) \leq 2$. (A thorough numerical investigation confirming this conclusion in the diffusion-only case is presented in Malham & Wiese (2009). Further, Lord *et al.* (2008) demonstrate that high accuracy, higher order stochastic integrators can deliver greater accuracy for a given computational effort, than the Euler–Maruyama scheme, despite the cost associated with simulating the multiple Wiener integrals included.) First we note that at this order, $\hat{\sigma}_{n,n+1}$ is also the form of the exponential Lie series for $g(w) \leq 2$ (this is not true at any higher orders) which is not an efficient integrator. However at this order, the two integrators are distinguished when we compute their inverse endomorphisms to generate the corresponding approximations. Second, the inverse of the sinhlog endomorphism is $\text{sinhlog}^{-1}(\sigma) = \sigma + (\text{id} + \sigma^2)^{1/2}$. If the vector fields are linear, $\hat{\sigma}_{n,n+1}$ is a matrix and we can construct $\text{sinhlog}^{-1}(\sigma)$ by computing the matrix square-root. If the vector fields are nonlinear we can expand the square root to sufficiently high degree terms (see Malham & Wiese 2009, Remark 5.3). Third, the stochastic Taylor based scheme above is a modification of the Milstein method where we additionally include terms involving J_{i0} , J_{0i} and J_{00} for $i = 1, \dots, d$.

We considered here a comparison under the mean-square measure of the local errors. How the local errors accumulate to contribute to the global error was considered in Malham & Wiese (2009), where it was shown that the local error comparison transfers to the global error.

If we know further structure in the stochastic differential system concerned, then the class of endomorphisms that are efficient will widen. For example, if the diffusion vector fields commute with themselves, but not with the drift vector field, then we can deduce that the exponential Lie series is (trivially) an efficient integrator, again, under the proviso we grade according to word length. This is because in the remainder at leading order, the largest terms according to root-mean-square scaling with respect to stepsize, will involve words with non-zero letters. However these will not in fact be present as the diffusion vector fields commute.

Our results have only relied on the symmetry properties of the expectation map (see Lemma 2) and that it realizes positive values on words with a scaling according to word length. In particular they do not depend on the coefficients explicitly. Hence the sinhlog integrator is optimally efficient within the whole class of possible coefficients. In a slightly different direction, our result also holds for weak approximations of the multiple integrals, as long as the L^2 -norm of (sums of) integrals is preserved. We assume here, that the error is still being measured in the mean-square sense.

Though in general the Eulerian idempotent is not efficient, it is a natural object in the construction of geometric integrators. Recently the Dynkin and Klyachko Lie algebra idempotents have proved to be important in the context of geometric integration, see Chapoton (2009), Patras & Reutenauer (2002), Munthe-Kaas & Wright (2007), and Lundervold & Munthe-Kaas (2011a,b). Interesting questions here besides the extension of their use to stochastic differential equations is which of these projectors generates a more accurate and efficient geometric integrator than the other?

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References

1. Azencott, R. 1982 Formule de Taylor stochastique et développement asymptotique d'intégrales de Feynman, Seminar on Probability XVI, *Lecture Notes in Math.* **921**, Springer, 237–285
2. Baudoin, F. 2004 *An introduction to the geometry of stochastic flows* Imperial College Press
3. Ben Arous, G. 1989 Flots et séries de Taylor stochastiques, *Probab. Theory Related Fields* **81**, 29–77

4. Buckwar, E., Malham, S.J.A. & Wiese, A. 2012 An introduction to SDE simulation, Preprint
5. Burgunder, E. 2008 Eulerian idempotent and Kashiwara–Vergne conjecture, *Annales de l’Institut Fourier* **58**(4), 1153–1184. doi: 10.5802/aif.2381
6. Castell, F. 1993 Asymptotic expansion of stochastic flows, *Probab. Theory Related Fields* **96**, 225–239
7. Castell, F. & Gaines, J. 1995 An efficient approximation method for stochastic differential equations by means of the exponential Lie series, *Math. Comp. Simulation* **38**, 13–19
8. Castell, F. & Gaines, J. 1996 The ordinary differential equation approach to asymptotically efficient schemes for solution of stochastic differential equations, *Ann. Inst. H. Poincaré Probab. Statist.* **32**(2), 231–250
9. Chen, K. T. 1957 Integration of paths, geometric invariants and a generalized Baker–Hausdorff formula, *Annals of Mathematics* **65**(1), 163–178
10. Chapoton, F. 2009 A rooted-trees q -series lifting a one-parameter family of Lie idempotents, *Algebra and Number Theory* **3**(6), 611–636
11. Ebrahimi–Fard, K. & Guo, L. 2006 Mixable shuffles, quasi-shuffles and Hopf algebras, *Journal of algebraic combinatorics* **24**(1), 83–101
12. Fliess, M. 1981 Fonctionnelles causales non linéaires et indéterminées non-commutatives, *Bulletin de la Société Mathématique de France* **109**, 3–40
13. Gaines, J. 1994 The algebra of iterated stochastic integrals, *Stochastics and Stochastics Reports* **49**, 169–179
14. Kloeden, P.E. & Platen, E. 1999 Numerical solution of stochastic differential equations, Springer
15. Levin, D. & Wildon, M. 2008 A combinatorial method for calculating the moments of the Lévy area, *Trans. AMS* **360**(12), 6695–6709.
16. Lord, G., Malham, S.J.A. & Wiese, A. 2008 Efficient strong integrators for linear stochastic systems, *SIAM J. Numer. Anal.* **46**(6), 2892–2919
17. Lundervold, A. and Munthe–Kaas, H. 2011a Hopf algebras of formal diffeomorphisms and numerical integration on manifolds, *Contemporary Mathematics* **539**, 295–324
18. Lundervold, A. and Munthe–Kaas, H. 2011b Backward error analysis and the substitution law for Lie group integrators, arXiv:1106.1071v1
19. Lyons, T. & Victoir, N. 2004 Cubature on Wiener space, *Proc. R. Soc. Lond. A*, **460**, 169–198
20. Lyons, T., Caruana, M. & Lévy, T. 2007 Differential equations driven by rough paths. École d’Été de Probabilités de Saint–Flour XXXIV-2004, Lecture Notes in Mathematics 1908, Springer
21. Magnus, W. 1954 On the exponential solution of differential equations for a linear operator, *Comm. Pure Appl. Math.*, **7**, 649–673
22. Malham, S.J.A., Wiese, A. 2008 Stochastic Lie group integrators, *SIAM J. Sci. Comput.* **30**(2), 597–617
23. Malham, S.J.A., Wiese, A. 2009 Stochastic expansions and Hopf algebras. *Proc. R. Soc. A* **465**, 3729–3749 doi:10.1098/rspa.2009.0203.
24. Malham, S.J.A., Wiese, A. 2011 Lévy area logistic expansion and simulation, arXiv:1107.0151v1
25. Manchon, D. 2008 Hopf algebras and renormalisation, *Handbook of algebra* **5** (M. Hazewinkel ed.), 365–427
26. Munthe–Kaas, H.Z. & Wright, W.M. 2008 On the Hopf algebraic structure of Lie group integrators, *Foundations of Computational Mathematics* **8**(2), 227–257
27. Newton, N.J. 1991 Asymptotically efficient Runge–Kutta methods for a class of Itô and Stratonovich equations, *SIAM J. Appl. Math.* **51**, 542–567
28. Patras, F. 1994 L’algèbre des descentes d’une bigèbre graduée, *J. Algebra* **170**, 547–566.
29. Patras, F., Reutenauer, C. 2002 On Dynkin and Klyachko idempotents in graded bialgebras, *Advances in Applied Mathematics* **28**, 560–579. doi:10.1006/aama.2001.0795
30. Reutenauer, C. 1993 *Free Lie algebras*, London Mathematical Society Monographs New Series 7, Oxford Science Publications
31. Strichartz, R.S. 1987 The Campbell–Baker–Hausdorff–Dynkin formula and solutions of differential equations, *J. Funct. Anal.* **72**, 320–345
32. Wiktorsson, M. 2001 Joint characteristic function and simultaneous simulation of iterated Itô integrals for multiple independent Brownian motions, *Ann. Appl. Probab.* **11**(2), 470–487